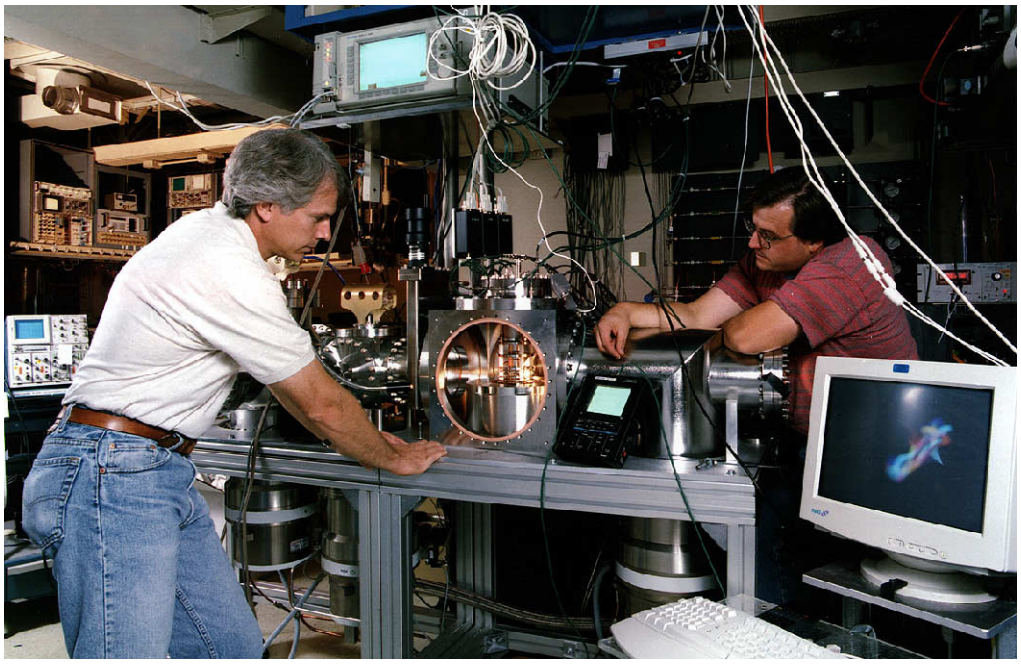
Combustion Chemistry

Fact Sheet

Capabilities/Selected Accomplishments:

- *Extensive use of multiple advanced laser diagnostics techniques, as well as state-of-the-art molecular beam sampling*
- *Use of a Sandia-developed ion-imaging technique to take "snapshots" of molecules colliding during chemical reactions, providing data on the velocities and state distributions of reaction products*
- *Use of ultrashort laser pulses to probe chemical events on the femtosecond time scale*
- *Use of pulsed photolysis/continuous-wave laser detection to measure rate constants and product distributions of individual chemical reactions*
- *Ability to predict rate coefficients and product distributions for elementary combustion reactions using quantum chemistry and dynamics calculations*
- *Ability to model the formation of combustion-generated pollution and to predict flame properties using Sandia-developed CHEMKIN software*
- *Developed mechanistic models for nitrogen oxide formation and destruction in combustion and for soot formation in combustion of aliphatic fuels*



Researchers assemble a new photoelectron/photoion imaging apparatus for use in femtosecond laser studies of fundamental chemical processes in isolated molecules.

Combustion Chemistry

Chemical transformations lie at the heart of combustion science. For example, pollution control requires a thorough understanding of pollutant formation chemistries and abatement strategies. Controlling engine knock also requires an in-depth understanding of the complex chemical processes of combustion.

The CRF conducts fundamental research in combustion chemistry, providing information needed to understand the complex chemical processes that occur when fuels burn. Sponsored by the Department of Energy's Office of Basic Energy Sciences, the program emphasizes determination of the rates and mechanisms of chemical reactions and the characterization of molecular structure and energetics. Scientists investigate chemical reactivity at varying levels of detail, from time-resolved studies of intramolecular processes to characterization of multi-reaction environments in combustion devices. The CRF maintains a vigorous research program in three principal subfields: chemical dynamics, chemical kinetics, and flame chemistry and combustion modeling.

Chemical Dynamics

Sandia's chemical dynamics research focuses primarily on gaining insight into how molecules undergo chemical change at the most detailed

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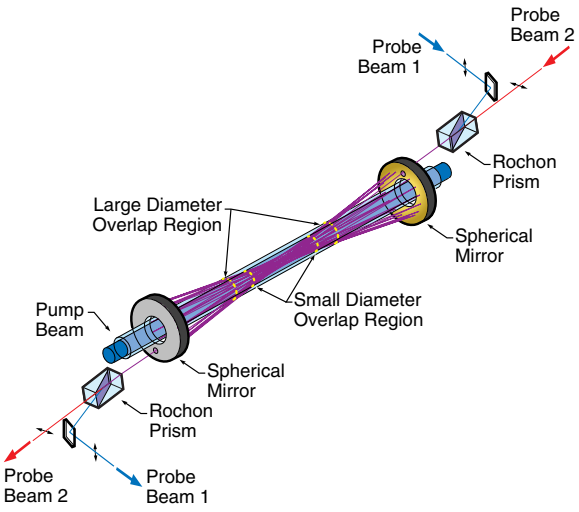
level. Research in this area emphasizes the interaction of light with molecules, intra- and intermolecular energy transfer, and uni- and bimolecular chemical reactions. Much of our work focuses on the spectroscopy, energetics, and dynamics of reactive species such as free radicals.

Chemical Kinetics

The goal of the chemical kinetics program is to understand the chemical processes that control combustion, specifically the microscopic mechanisms involved in individual chemical transformations, the rates at which they proceed, and the products they produce. We can then improve our knowledge of how flames burn, why engines knock, and how to minimize pollution.

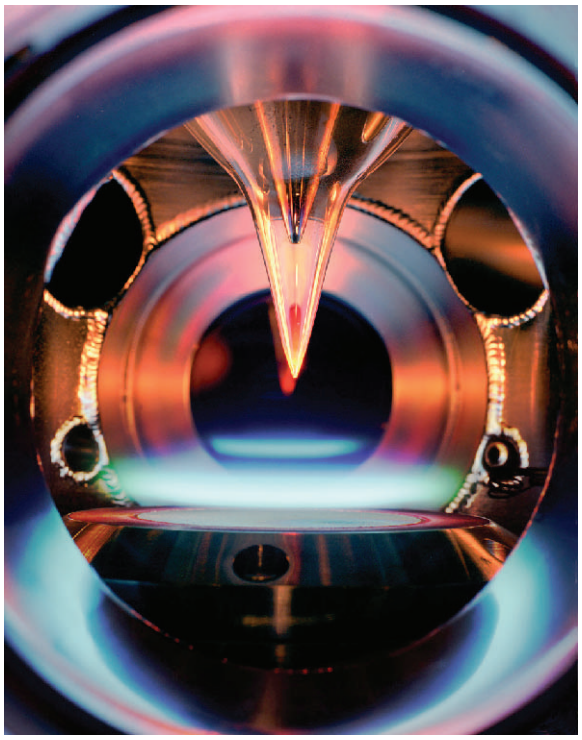


Schematic drawing of the optical configuration used to study the rates and mechanisms of chemical reactions important in combustion.

Flame Chemistry and Combustion Modeling

The goal of this research is to explain the chemical mechanisms of combustion through a combination of experiments based on state-of-the-art diagnostics and and detailed chemical kinetic modeling. The experimental program concentrates on the development and application of combustion diagnostics for measuring the concentration of the key chemical species that are produced and destroyed during combustion.

Research in combustion modeling focuses primarily on the pathways involved in hydrocarbon oxidation and in the formation and control of pollutants such as nitrogen oxides and soot. The computational techniques used range from calculating the details of molecular electronic structure and dynamics to modeling the chemical kinetics of flames.



Low-pressure, flat -flames are used to investigate combustion chemistry in model systems. A variety of laser and mass spectrometer diagnostics are employed to measure the concentration of chemical intermediates throughout the flame. Pictured above the blue methane flame is a quartz sampling probe which forms the input into the molecular-beam mass spectrometer.

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